Overview of IH-related Projects @ Los Alamos National Laboratory

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National Nuclear Security Administration

Los Alamos NATIONAL LABORATORY

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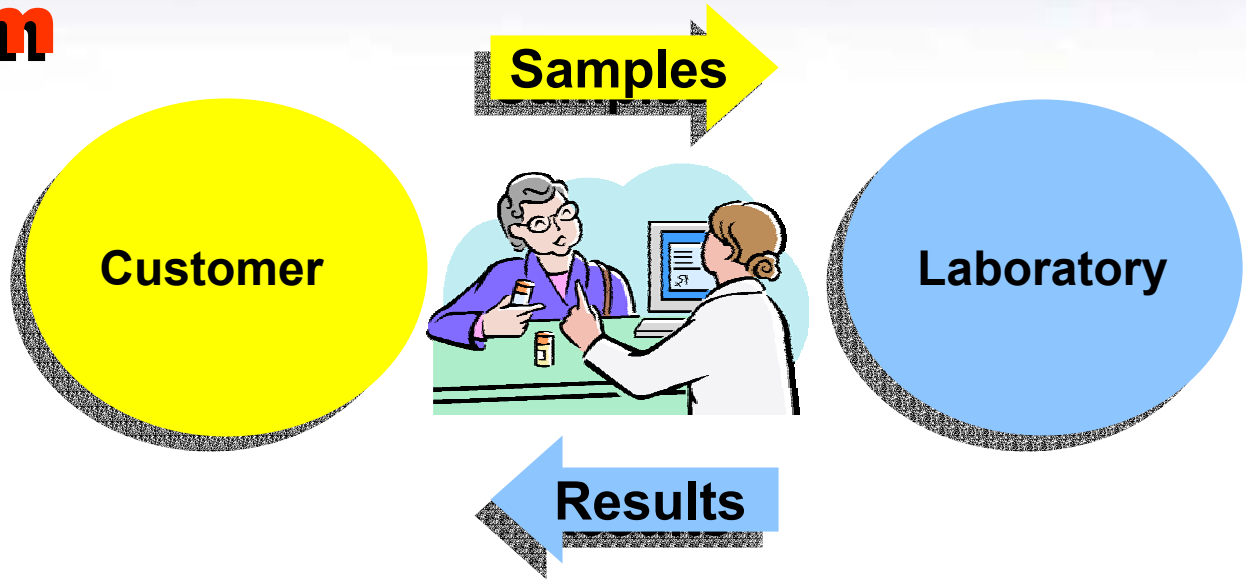
Agenda

- Automating IH Records Management and Data Exchange
- Automated Instrument Data QC
- Handheld Sample Collection & Tracking Device

Automating IH Records Management and Data Exchange

The Problem



- Use of paper forms (time consuming, requires manual validation, error prone due to re-keying, duplication of effort)
- No direct data import/export capabilities between different systems

Automating IH Records Management and Data Exchange

Our Goal

Develop data models and an information portal that enables lab- and IH folks to exchange information electronically in a platform- & system-independent manner.

Automating IH Records Management and Data Exchange

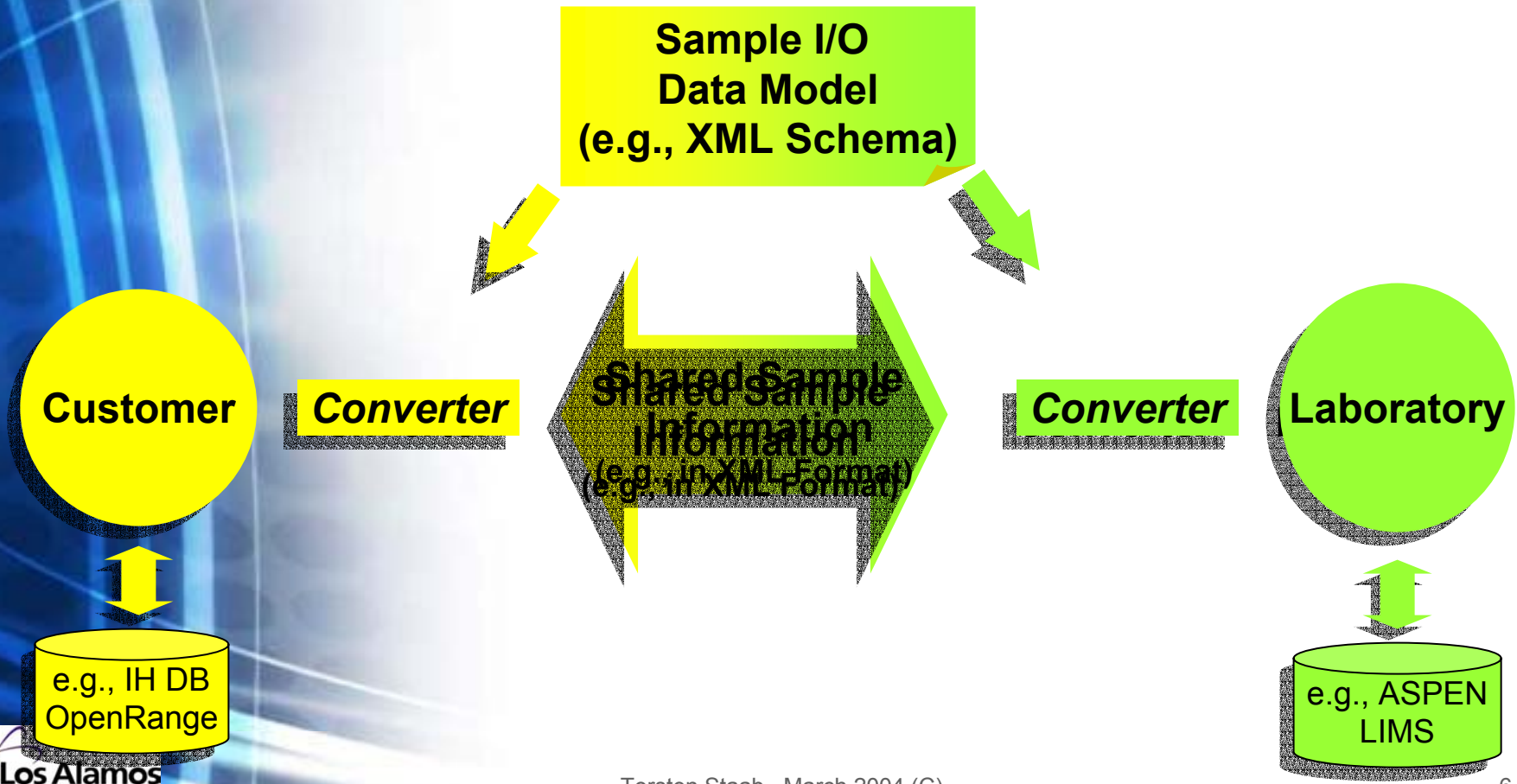
Our Approach

- Platform-neutral Data Modeling and Representation using **XML** (eXtensible Markup Language)
- Automate Records Management, Tracking, Approval, and Routing with **Microsoft Sharepoint**

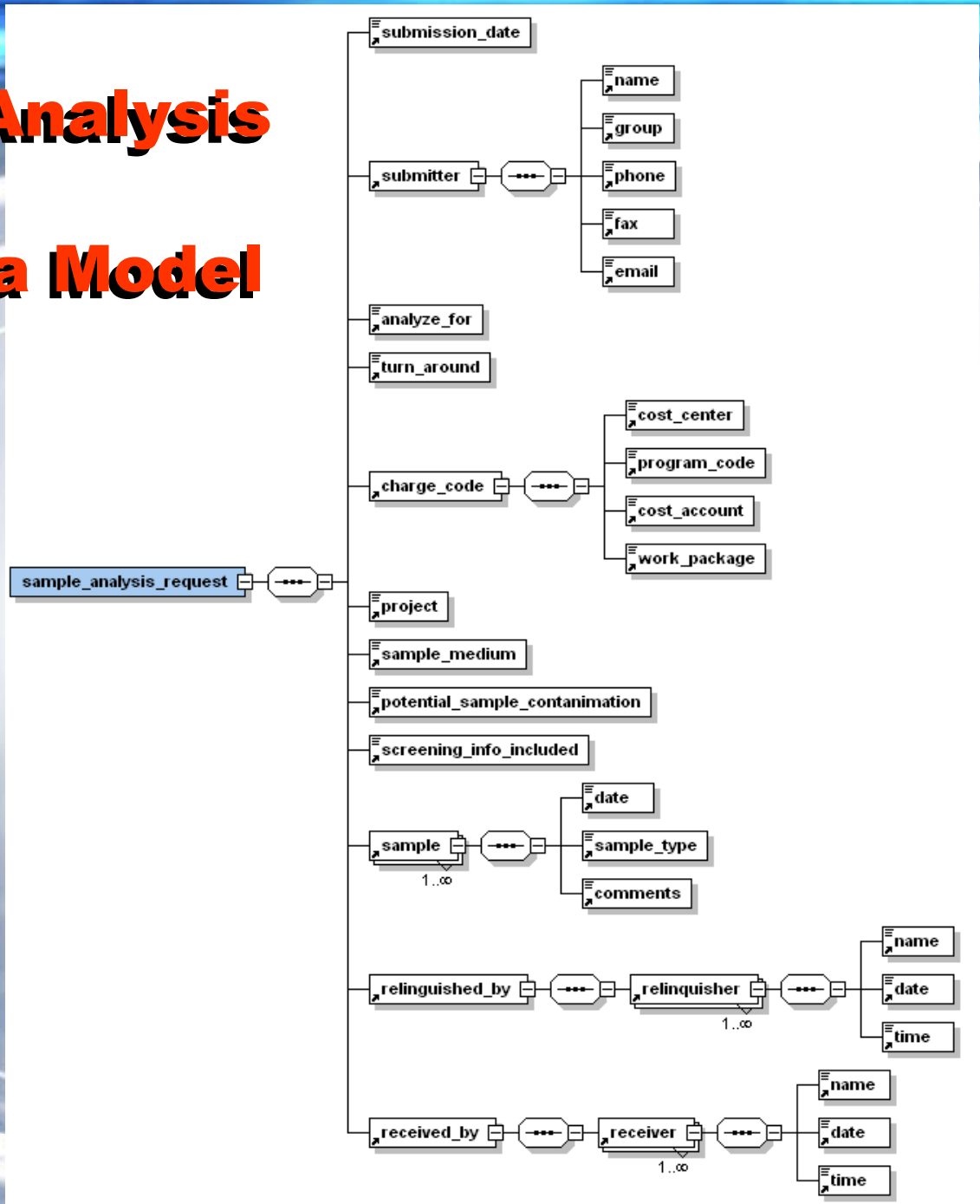
visit http://www.w3.org/XML/ for more info on XML

Automating IH Records Management and Data Exchange

System Architecture

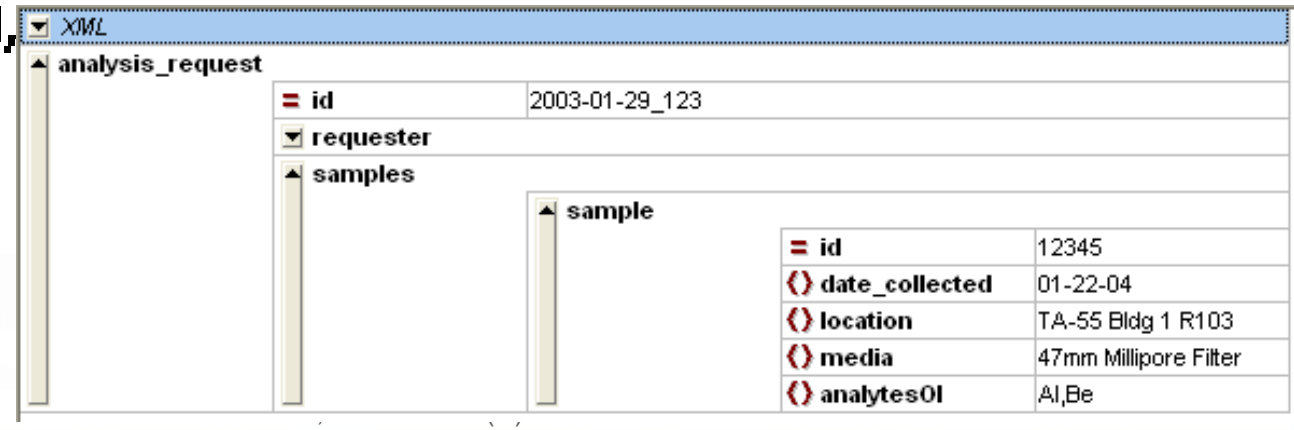


Sample Analysis Request XML Data Model



Sample Analysis Request XML Example

```
<?xml version="1.0" encoding="UTF-8" ?>
- <analysis_request id="2003-01-29_123">
  - <requester>
      <name>Alice Smith</name>
      <group>MST-6</group>
    </requester>
  - <samples>
    - <sample id="12345">
        <date_collected>01-22-04</date_collected>
        <location>TA-55 Bldg 1 R103</location>
        <media>47mm Millipore Filter</media>
        <analytesOI>Al,
      </sample>
    </samples>
  </analysis_request>
```



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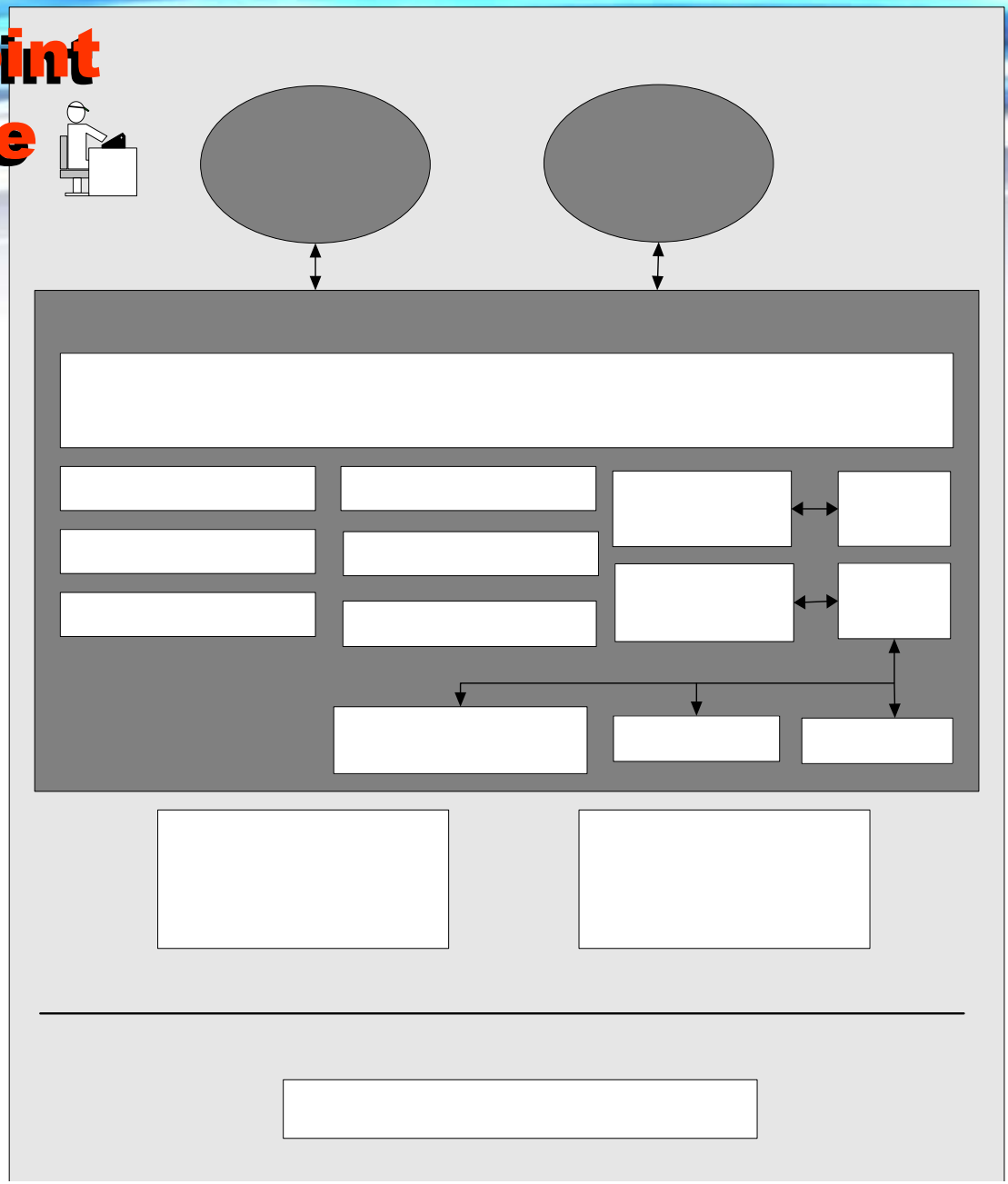
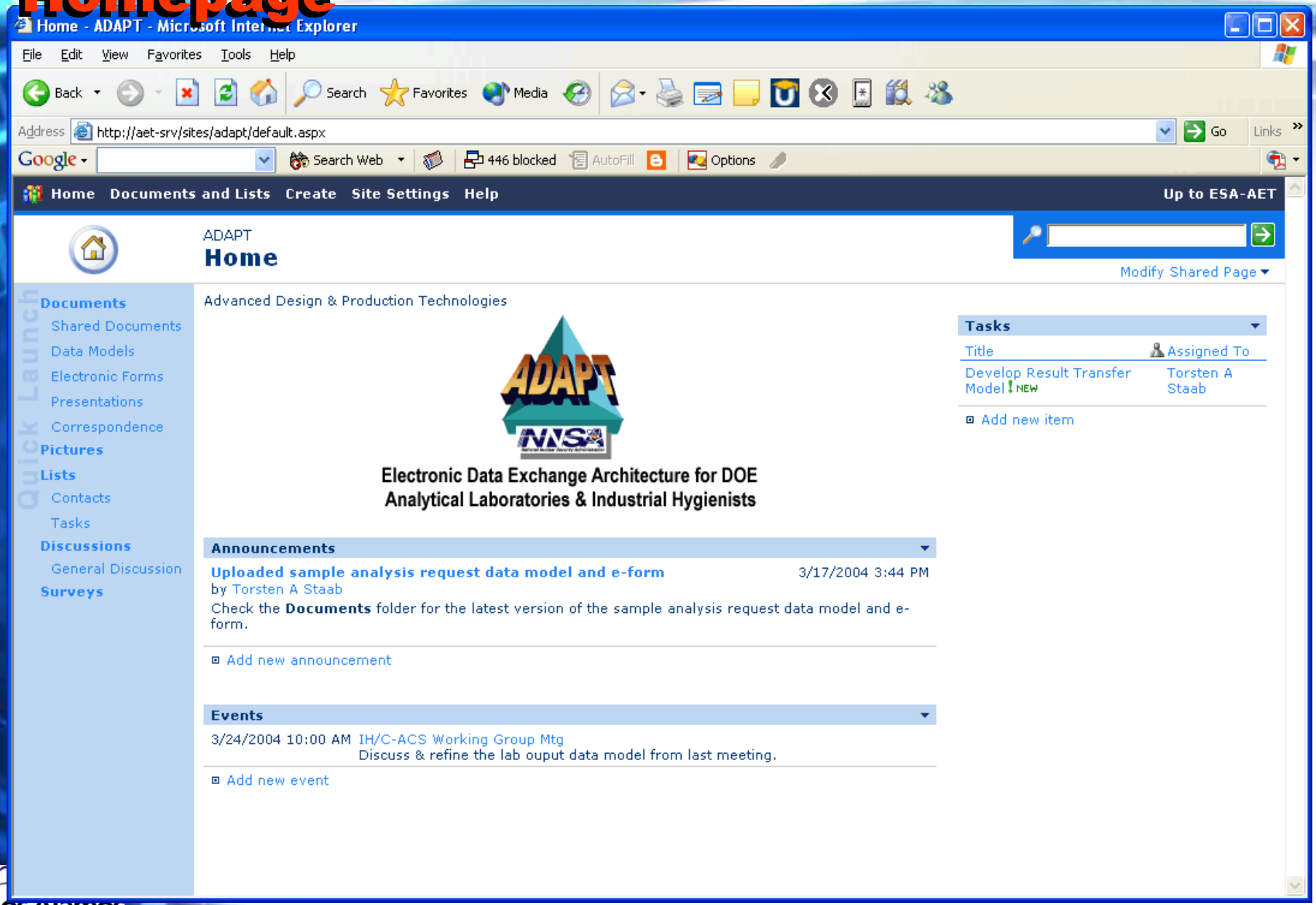
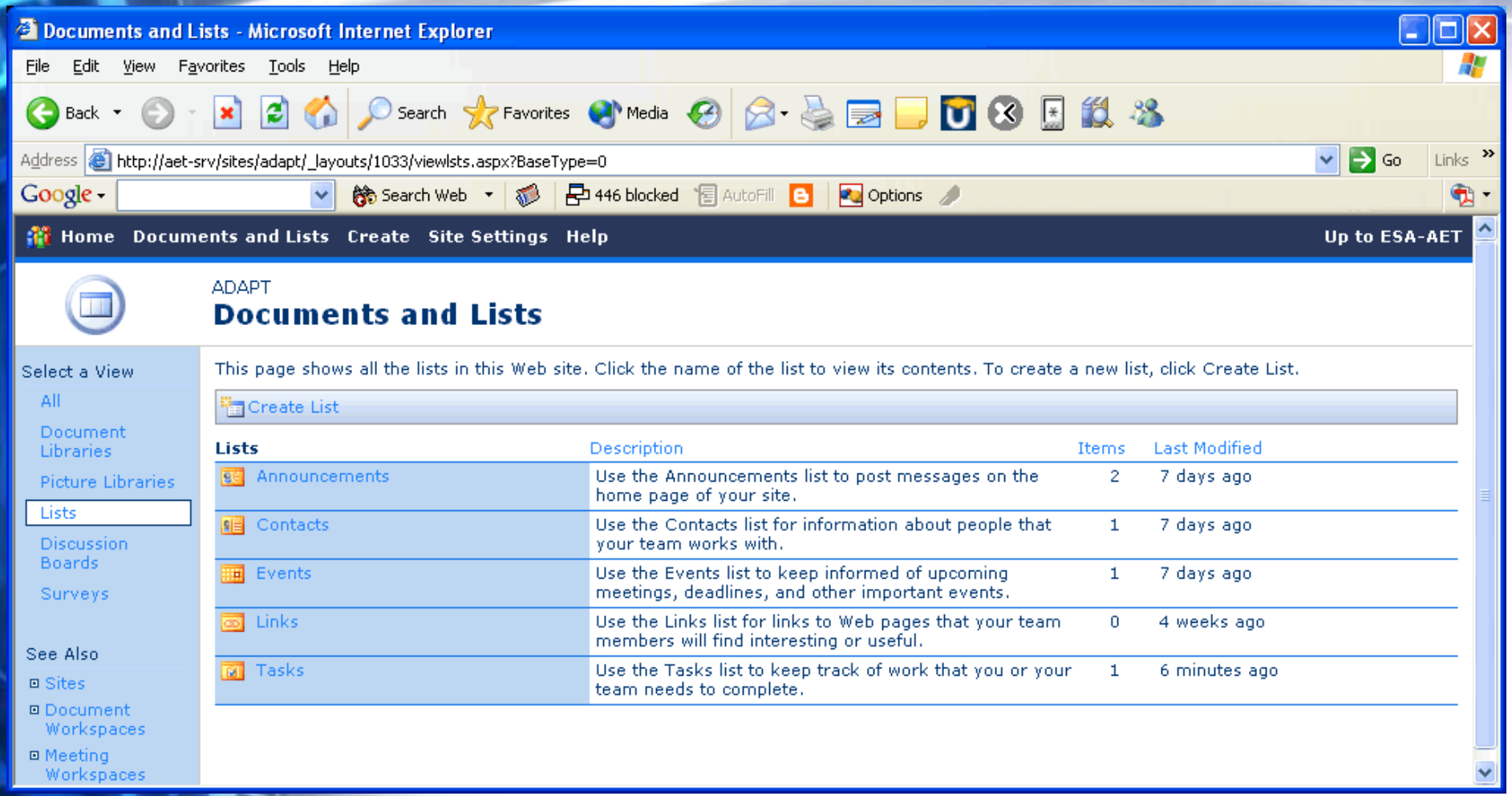
Microsoft Sharepoint Portal Architecture



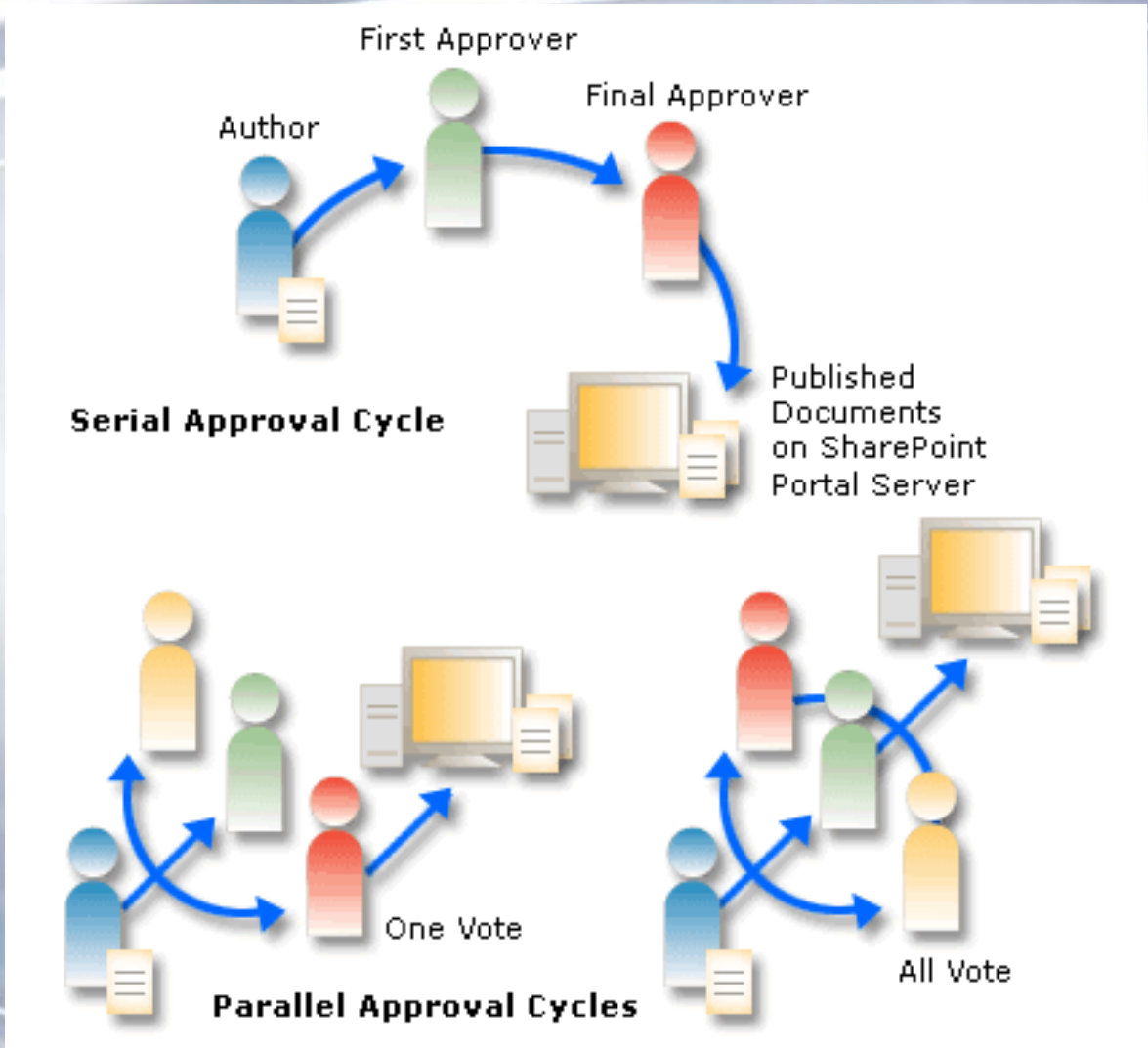
Example: ADAPT Project Sharepoint Homepage



ADAPT Project Sharepoint Documents & Lists

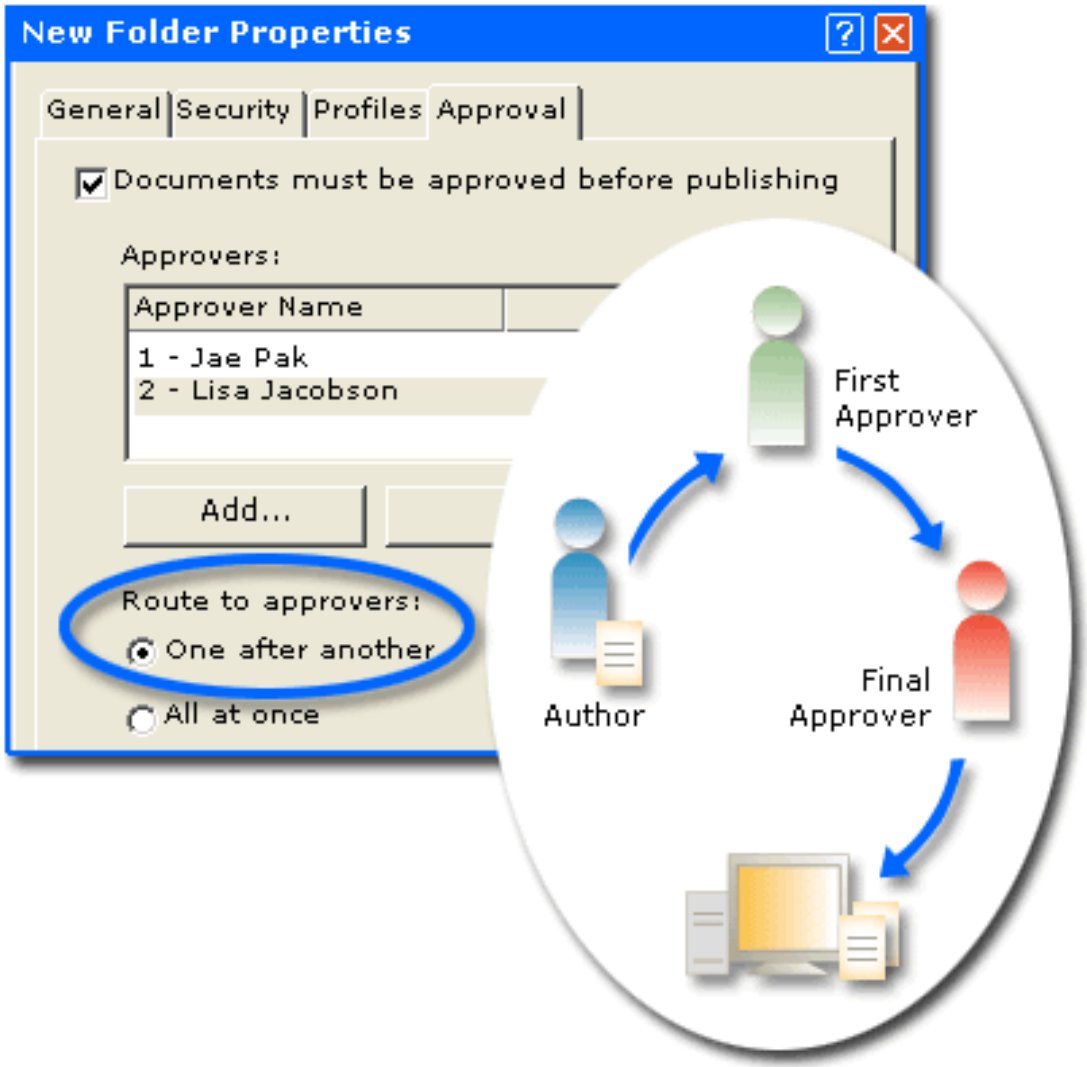


Document Approval Cycle Types in Sharepoint

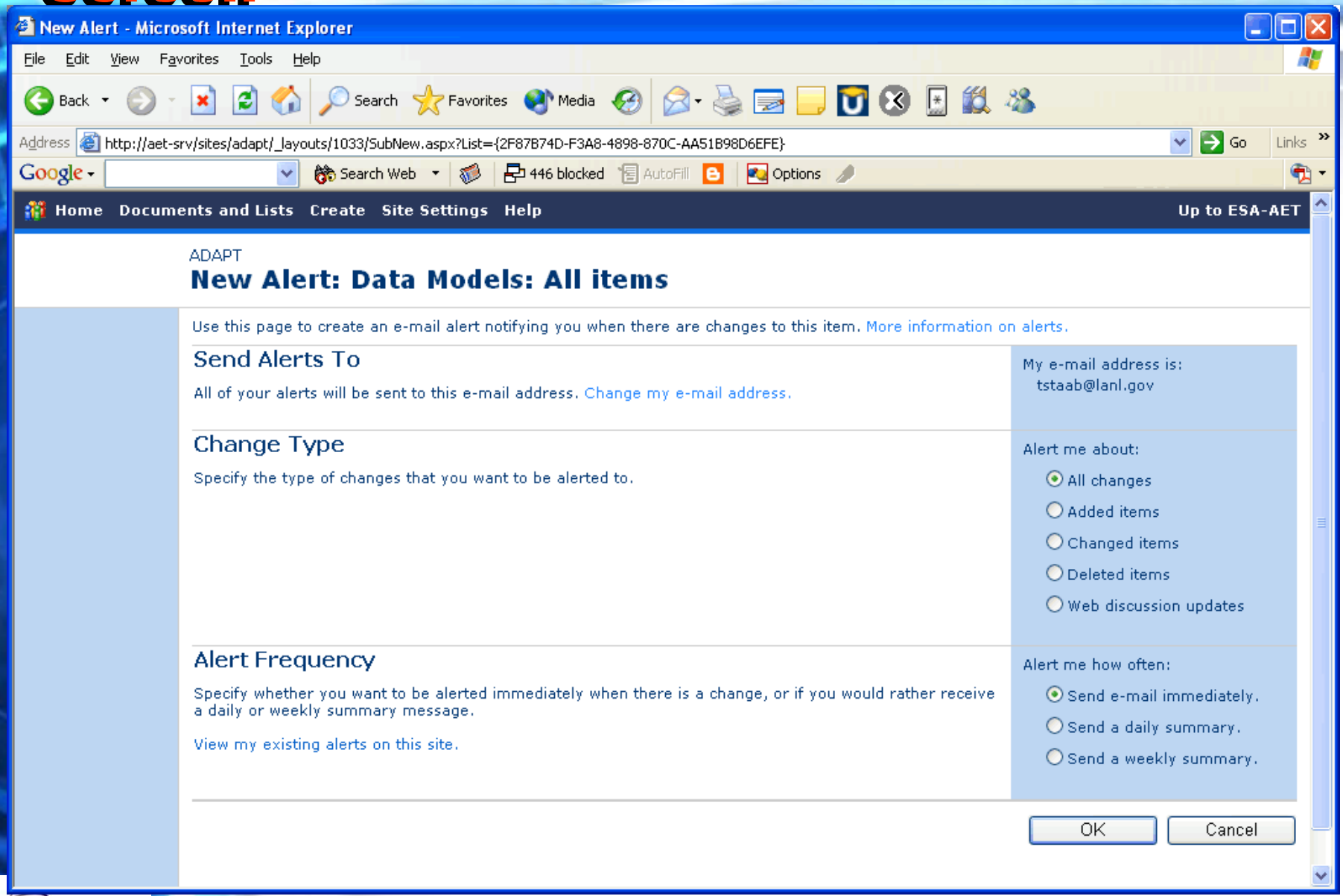


Approval Routing Setup in Sharepoint

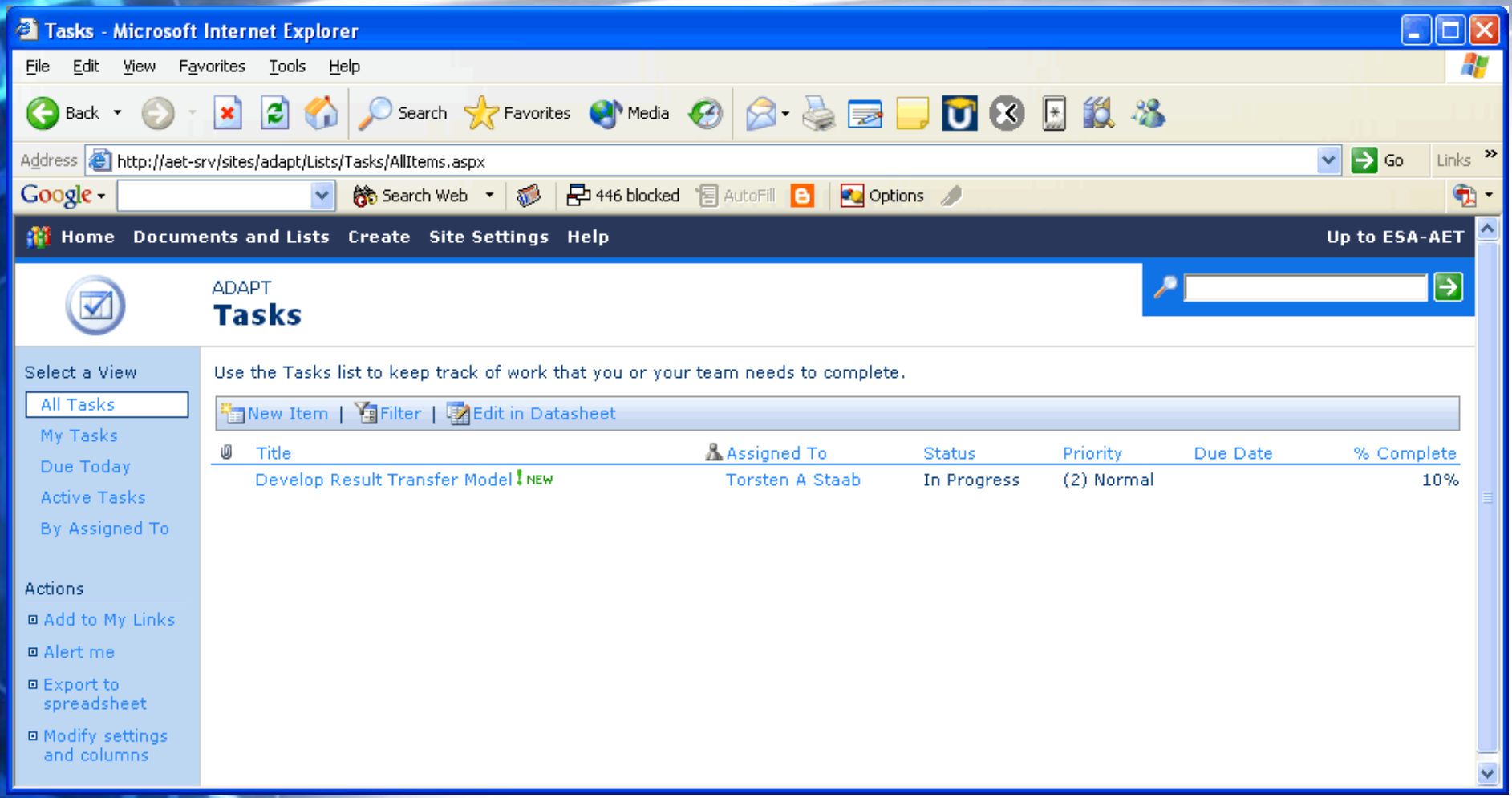
As a coordinator on a folder, you can choose the approval route.



ADAPT Project Sharepoint New Alert Screen



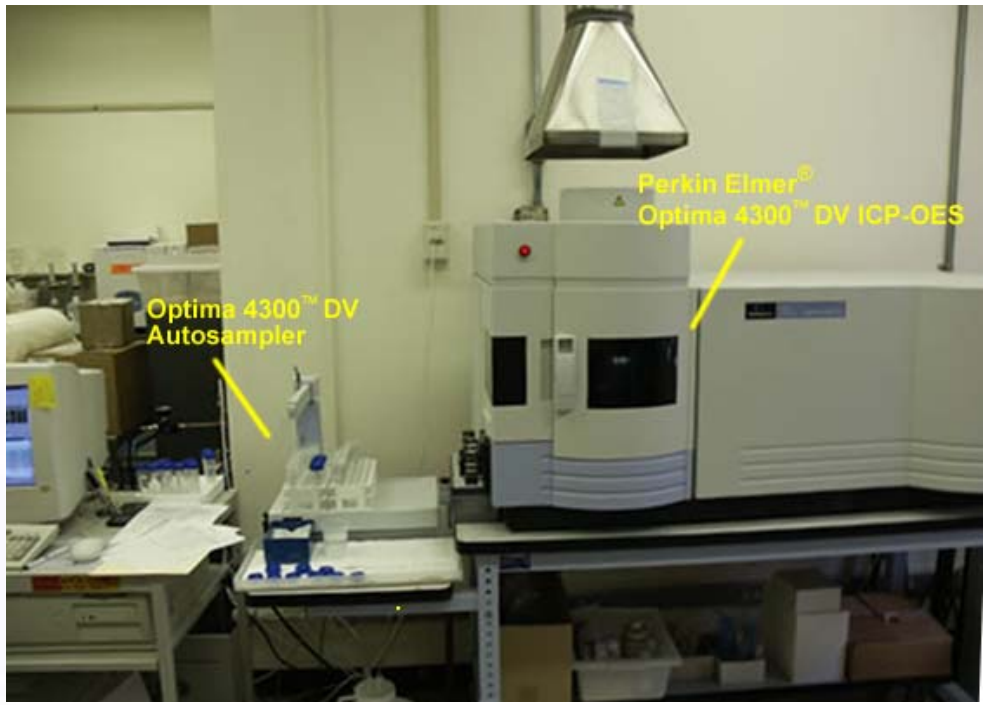
ADAPT Project Sharepoint Tasks Screen



Automating Instrument Data QC

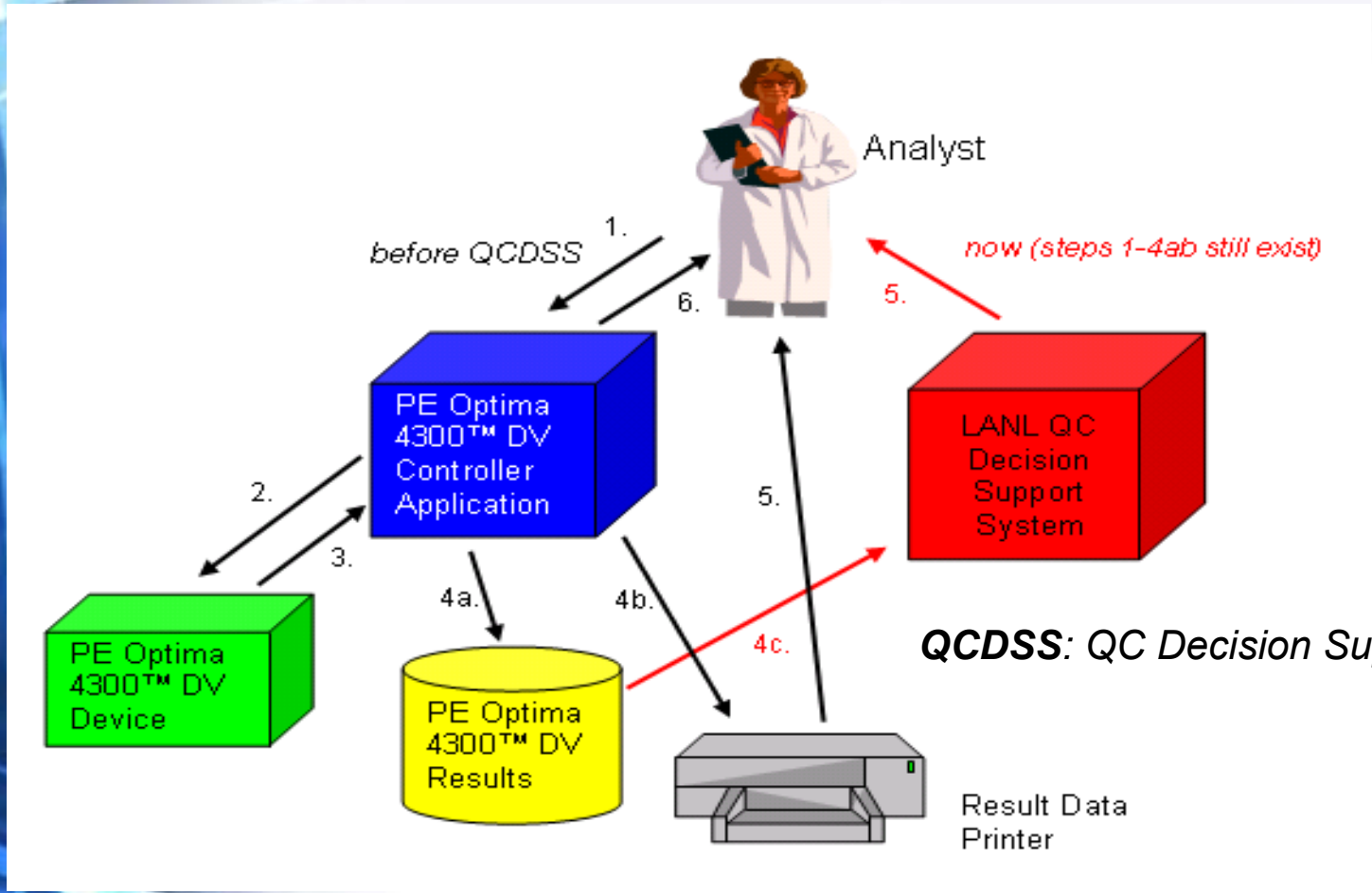
The Goal

Automate labor-intensive and time-consuming QC of instrument-generated analysis result data



Automating Instrument Data QC

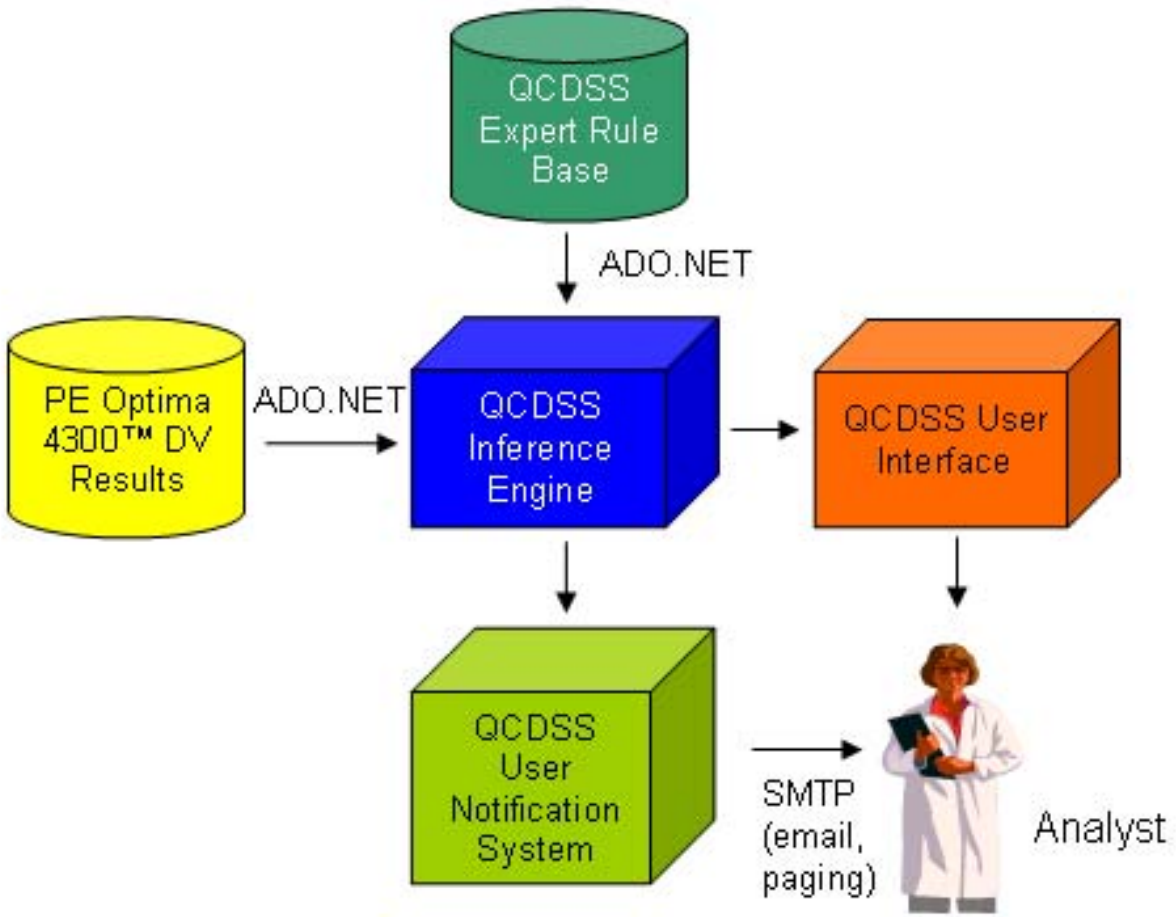
The System Architecture (1/2)



***QCDSS**: QC Decision Support System*

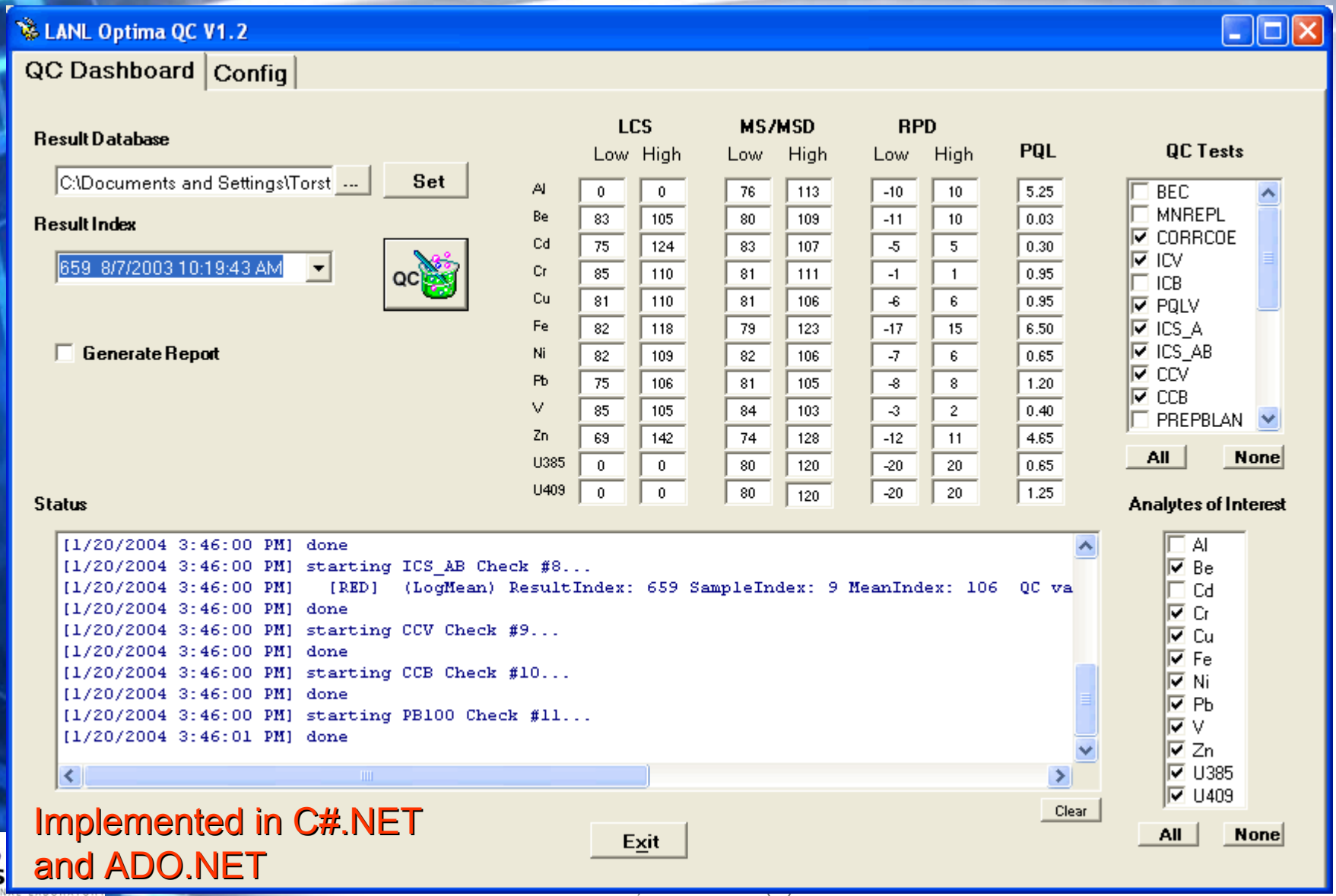
Automating Instrument Data QC

The System Architecture (2/2)



Automating Instrument Data QC

Screenshot of Software Prototype



Implemented in C#.NET and ADO.NET

QCDSS-generated, HTML-based QC Report

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Analyst Checklist

C-ACS IH Team

Prep Batch ID:	113	Analytes Requested:	Al, Cu, Fe	Results DataSet:	100
SDG#:	A34	Sample Type:	Metals	Analysis Date:	11/3/2003
Sample ID#s:	123, 456, 789			Analyst:	Torsten

Acceptance Limits

Analyte	LCS	MS_MSD	RPD	PQL
Al	N/A	76-113	(-10) – (+10) %	5.25
Be	83-105	80-109	(-11) – (+10) %	0.03
Cd	75-124	83-107	(-5) – (+5) %	0.30
Cr	85-110	81-111	(-1) – (+1) %	0.95
Cu	81-110	81-106	(-6) – (+6) %	0.95
Fe	82-118	79-123	(-17) – (+15) %	6.50
Ni	82-109	82-106	(-7) – (+6) %	0.65
Pb	75-106	81-105	(-8) – (+8) %	1.20
V	85-105	84-103	(-3) – (+2) %	0.40
Zn	69-142	74-128	(-12) – (+11) %	4.65
U385	N/A	80-120	(-20) – (+20) %	0.65
U409	N/A	80-120	(-20) – (+20) %	1.25

Tests

Description	Passed	Failed
1) Did BEC check pass (< 0.04)?	×	
2) Did Mn replicate test pass (< 2.0% RSD)?	×	
3) Is Correlation Coefficient >/= 0.9950		×
4) Did ICV pass (90-110%)?	×	
5) Did ICB pass (-1 to 3x PQL)?		×
6) Did PQLV pass (70-130%)?	×	
7) Did ICS_A pass (-1 to 3x PQL)?	×	
8) Did ICS_ AB pass (80-120%)?		×
9) Did CCV pass (90-110%)?	×	
10) Did CCB pass (-1 to 3x PQL)?		×
11) Did Prep Blank pass (-1 to 3x PQL)?	×	
12) Did Media Blank pass (-1 to 3x PQL)?	×	
13) Did LCS pass?		×
14) Did MS recovery pass?	×	
15) Did MSD recovery pass?		×
16) Did MSD RPD pass?	×	
17) Were standards and solutions current?	×	
18) Did PB100 pass?		×
19) Did Real Sample Measurement pass?	×	
20) Did Rinse Blank pass?	×	

Standard Prep. Logbook ID#/Page:

Prepared by:

Date prepared:

If "Failed" is checked, reference the number and describe the problem below:

- Be oversaturated
- Al without limits

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Automating Instrument Data QC

Results of Automating Instrument QC

- LANL program performs QC in ~5 seconds as opposed to 20 minutes needed by human analyst
- improves sample analysis QC by eliminating potential for human error
- reduces laboratory operating cost; saves one Tech FTE per instrument per year
- minimizes device downtime and saves resources through a built-in, real-time, electronic notification system
- speeds up reporting by generating QC reports on-the-fly

Automating Instrument Data QC

Future Work

- apply same QC automation framework to other instruments
- store meta description of expert rules in a database and generate decision support system on-the-fly from stored rules
- LIMS Integration

Recent Paper: ***Improving Sample Analysis Throughout and Quality with a .NET-based, Real Time QC Decision Support System***, Torsten Staab, Toshiyuki Shiina, Derek Miller, Journal of the Association for Laboratory Automation (JALA), Elsevier Publishers, Vol 8/6, pp 107-112, December 2003.

Handheld Sample Collection & Tracking Device

The Goals

- speed up indoor and outdoor sample collection (e.g., surface swipes with filter papers, contact plates, swabs, etc.) and minimize human error by automating the book keeping
- allow for cross contamination-free sampling
- minimize risk of human contact exposure
- reduce sampling costs

Handheld Sample Collection & Tracking Device

Technology Summary

Handheld device for multi-purpose indoor and outdoor sample collection & electronic sample registration.

1st Generation Prototype

Technology Components

- PDA / Wearable Computer
- Universal Sample Media Adapter
- Built-in Digital Camera
- 3D Location Tracking
- GPS
- Wireless Communication
- Voice Control
- Pressure Sensor etc.